Comparative evaluation of electro-oxidation coupled with UV irradiation (UV/EO) and conventional oxidation processes (UV irradiation, chlorination, electro-oxidation, UV/Chlorine) for atenolol removal: Role of operating parameters, energy performance, and toxicity

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Supplementary information

Supplementary text-1 •OH and •Cl calculation

•OH concentration

$$\frac{d[pCBA]}{dt} = -k_{pCBA-\bullet OH}[\bullet OH][pCBA] \quad (1)$$

Comparing with the pseudo 1st-order equation for pCBA removal,

$$k'_{pCBA} = k_{pCBA-\bullet OH}[\bullet OH] \quad (2)$$

where $k_{pCBA-\bullet OH}$ is the 2nd-order reaction rate constant for pCBA with •OH (5×10^{9} $M^{-1}s^{-1}$) (Rosenfeldt, Linden, Canonica, & von Gunten, 2006). k'_{pCBA} is the observed kinetic data of pCBA removal (pseudo 1st-order degradation rate constant). [•OH] and [pCBA] are concentrations of •OH and pCBA, respectively.

Substitute the k'_{pCBA} of 0.0220 min^{-1} or 3.67×10^{-4} s^{-1} in the equation 2,

$$3.67 \times 10^{-4}\ s^{-1} = 5.00 \times 10^{9}\ M^{-1}s^{-1} \times [\bullet OH]$$

$$\text{Thus,} \quad [\bullet OH] = 7.34 \times 10^{-14}\ M$$

RCS concentration

$$\frac{d[BA]}{dt} = -\left(k_{BA-\bullet OH}[\bullet OH] + k_{BA-Cl\bullet}[Cl\bullet]\right).[BA] \quad (3)$$

Comparing with the pseudo 1st-order equation for BA removal,

$$k'_{BA} = k_{BA-\bullet OH}[\bullet OH] + k_{BA-Cl\bullet}[Cl\bullet] \quad (4)$$

where $k_{BA-\bullet OH}$, and $k_{BA-Cl\bullet}$ are 2nd-order reaction rate constants for BA with •OH (5.9×10^{9} $M^{-1}s^{-1}$) and BA with Cl• (1.8×10^{10} $M^{-1}s^{-1}$), respectively (Wang, Wu, Huang, Wang, & Hu, 2016; Hoang, et al., 2022). k'_{BA} is the observed kinetic data of BA degradation (pseudo 1st-order degradation rate constant). [•OH] and [Cl•] are amount of •OH and Cl•, respectively.

Substitute the k'_{BA} of 0.0286 min^{-1} or 4.77×10^{-4} s^{-1} in the equation 4,

$$4.77 \times 10^{-4}\ s^{-1} = (5.90 \times 10^{9}\ M^{-1}s^{-1})\ (7.34 \times 10^{-14}\ M) + 1.80 \times 10^{10}\ M^{-1}s^{-1}[Cl\bullet]$$

Thus, $[Cl\bullet] = 2.42 \times 10^{-15}$ M

Supplementary text-2 Calculation of kinetic degradation rate of ATL by Cl• ($\boldsymbol{k_{ATL\text{-}Cl\bullet}}$)

$$\frac{d[ATL]}{dt} = -(k_{\bullet OH}[\bullet OH] + k_{Cl\bullet}[Cl\bullet] + k_{FAC}[FAC] + k_{UV}[\Phi I])[ATL] \quad (5)$$

Comparing with the pseudo 1st-order kinetic model of ATL removal,

$$k'_{UV/EO\text{-}ATL} = k_{\bullet OH}[\bullet OH] + k_{Cl\bullet}[Cl\bullet] + k_{FAC}[FAC] + k_{UV}[\Phi \varepsilon I] \quad (6)$$

$$k'_{FAC\text{-}ATL} = k_{FAC}[FAC] \quad (7)$$

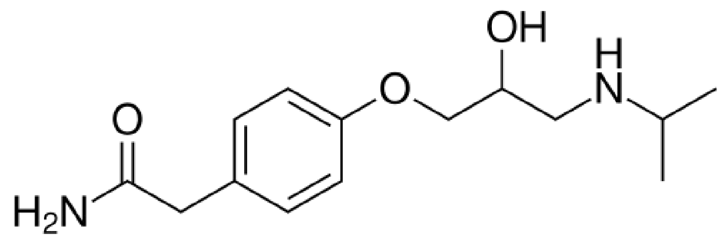
$$k'_{UV\text{-}ATL} = k_{UV}[\Phi \varepsilon I] \quad (8)$$

where $k'_{UV/EO\text{-}ATL}$, $k'_{FAC\text{-}ATL}$, and $k'_{UV\text{-}ATL}$ are the observed kinetic data of ATL degradation by the UV/EO process, chlorination, and UV irradiation, respectively. $k_{\bullet OH}$, $k_{Cl\bullet}$, k_{FAC}, and k_{UV} are 2nd-order reaction rate constants of ATL to •OH, Cl•, FAC, and UV light, respectively. [•OH], [Cl•], and [FAC] are concentrations of •OH, Cl•, and FAC, respectively. Φ, ε, and I are quantum yield of ATL, molar absorption of ATL, and the UV fluence rate, respectively.

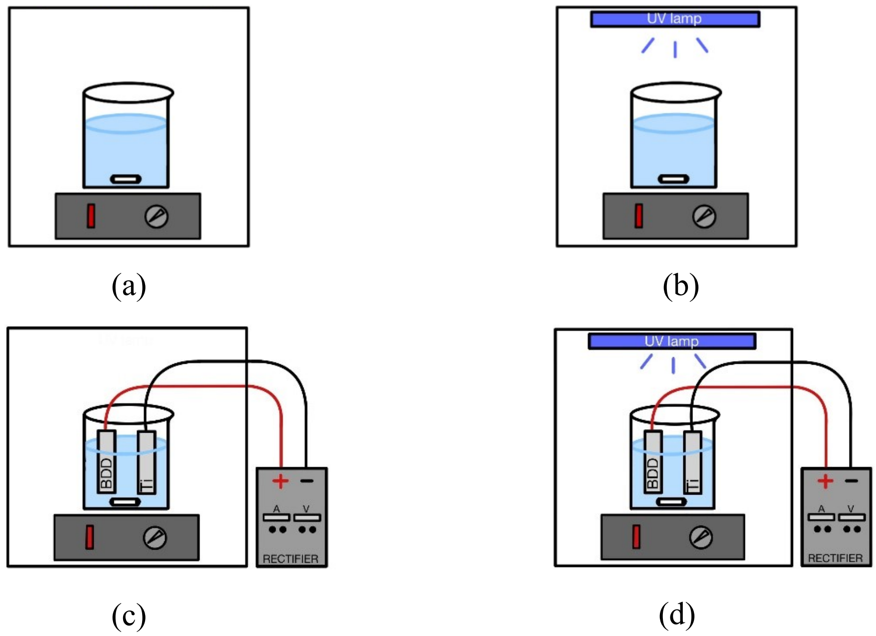
From the supplementary figure-1, $k'_{UV/EO\text{-}ATL}$, $k'_{UV\text{-}ATL}$, and $k'_{FAC\text{-}ATL}$ were 0.0599 min^{-1} (9.98×10^{-4} s^{-1}), 0.0025 min^{-1} (4.17×10^{-5} s^{-1}), 0.0035 min^{-1} (5.83×10^{-5} s^{-1}), respectively. $k_{\bullet OH\text{-}ATL}$ was 7.10×10^{9} $M^{-1}s^{-1}$ (Wols, Harmsen, Beerendonk, & Hofman-Caris, 2014). Substitute all values in the equation 6;

$$9.98 \times 10^{-4}\ s^{-1} = (7.10 \times 10^{9}\ M^{-1}s^{-1})(7.34 \times 10^{-14}\ M) + k_{Cl\bullet}(2.42 \times 10^{-15}\ M) + (5.83 \times 10^{-5}\ s^{-1}) + (4.17 \times 10^{-5}\ s^{-1})$$

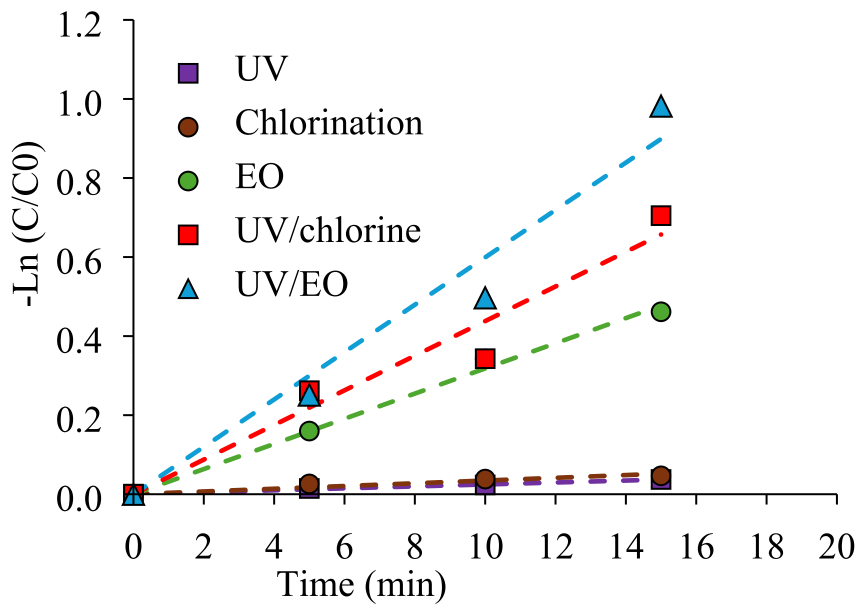
$$k_{Cl\bullet\text{-}ATL} = 1.55 \times 10^{11}\ M^{-1}s^{-1}$$



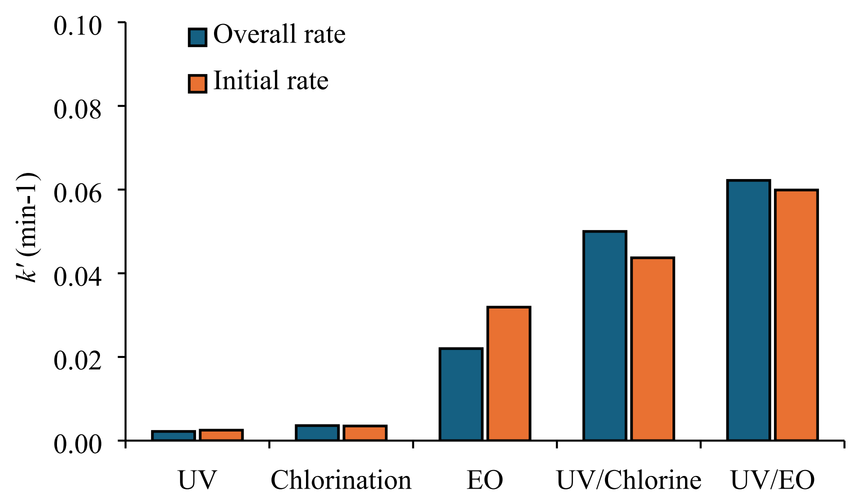
Supplementary figure-1 ATL structure



Supplementary figure-2 Experimental setup (a) Chlorination, (b) UV irradiation and UV/chlorine, (c) EO process, and (d) UV/EO process

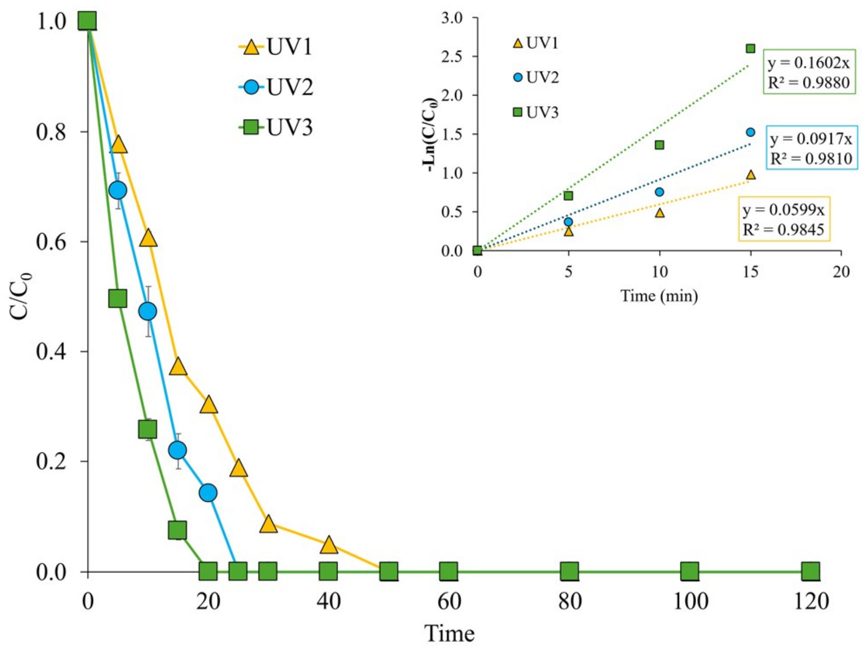


(a)

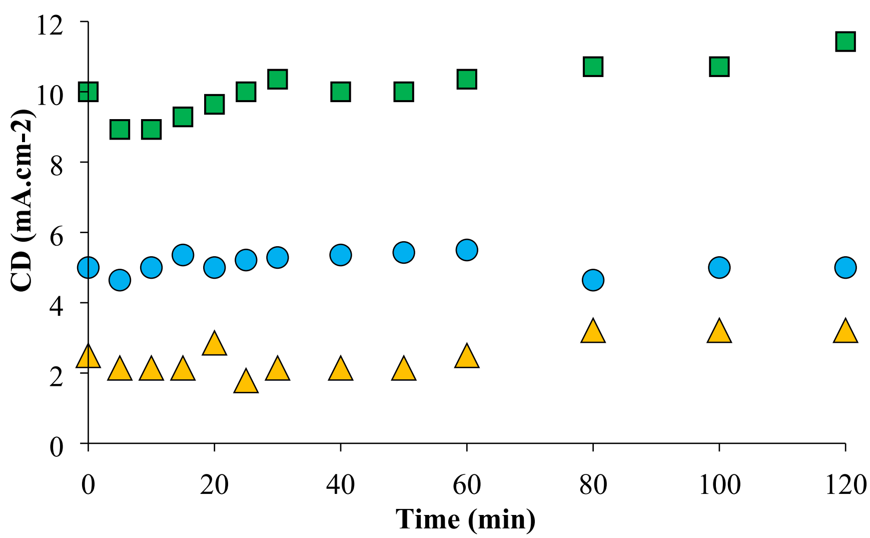


(b)

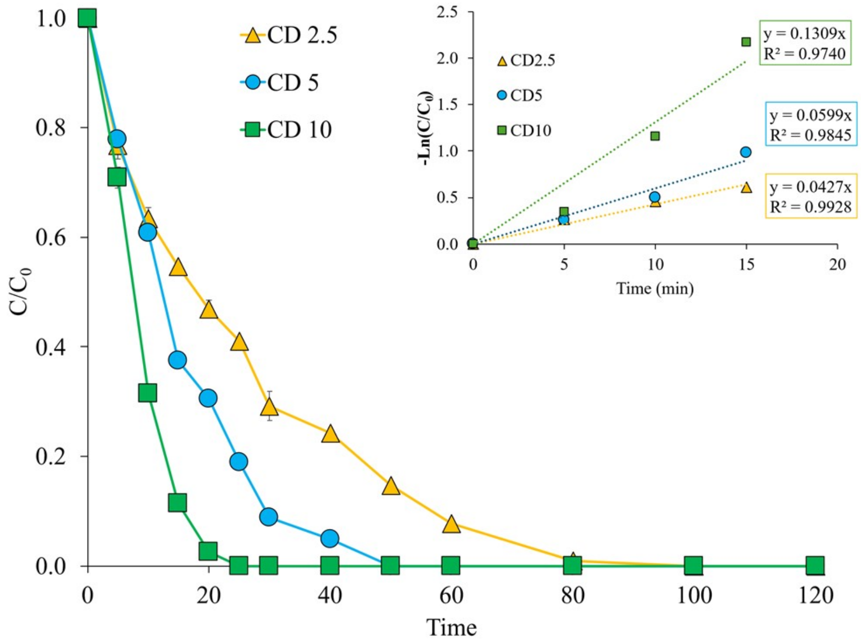
Supplementary figure-3 Kinetic ATL degradation by the initial rate method (a) and overall rate (b) for chlorination, UV irradiation, EO, UV/Chlorine, and UV/EO



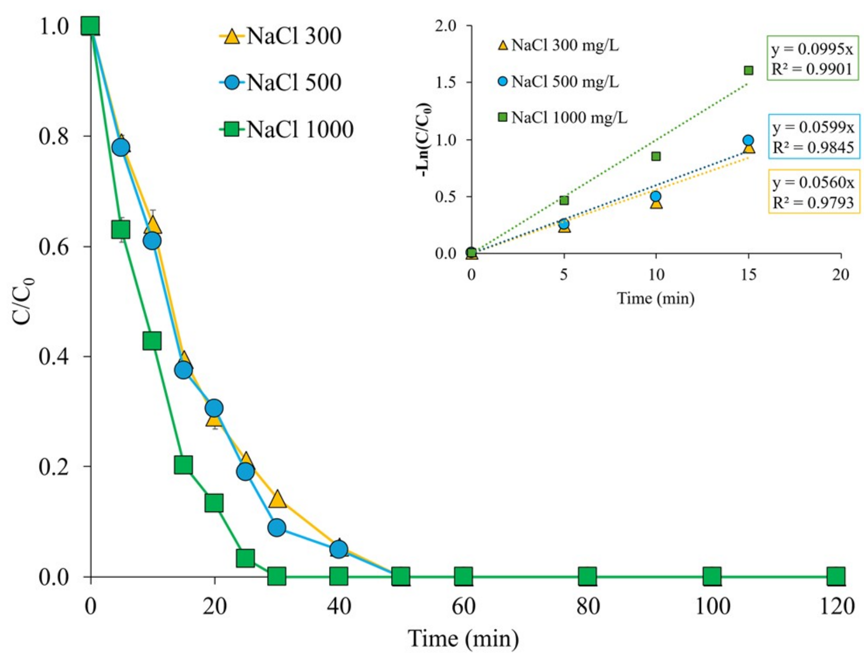
Supplementary figure-4 Effect of UV lamp on kinetic degradation of ATL in UV/EO



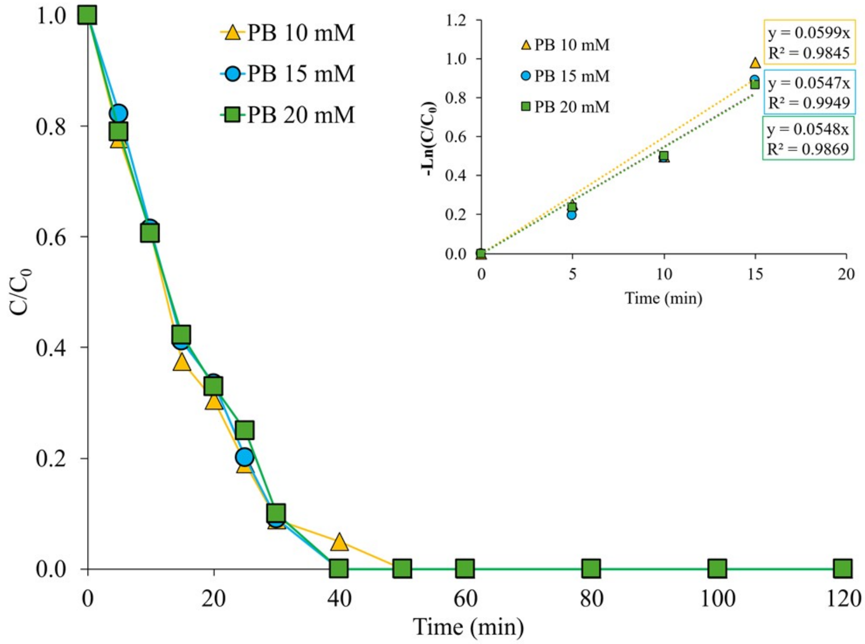
Supplementary figure-5 The CD profile of UV/EO



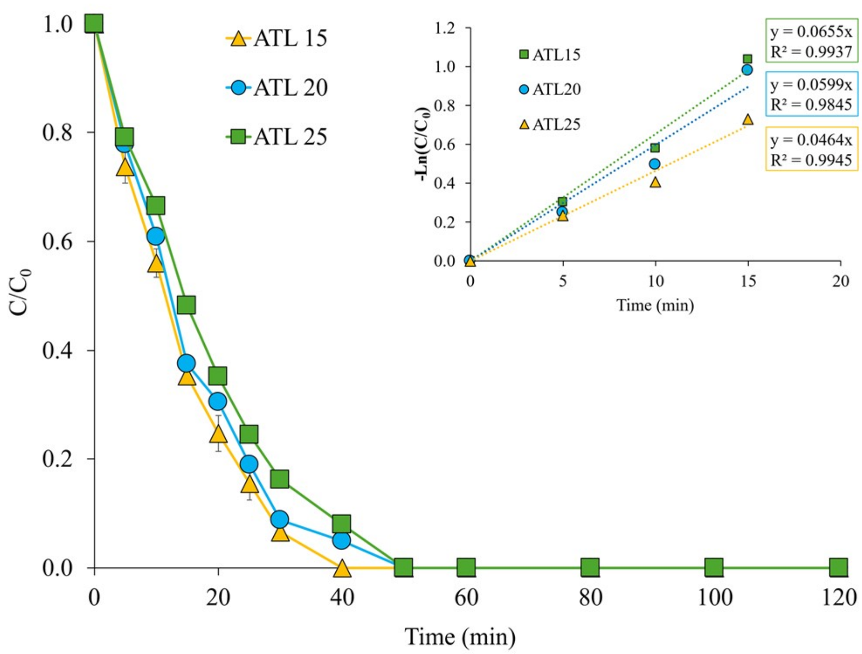
Supplementary figure-6 Effect of CD on kinetic degradation of ATL in UV/EO



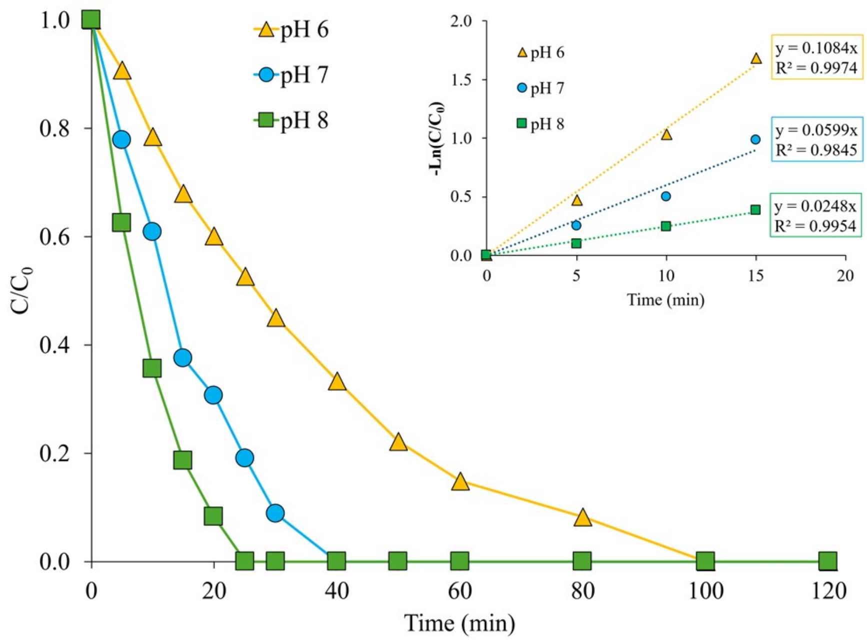
Supplementary figure-7 Effect of NaCl on kinetic degradation of ATL in UV/EO



Supplementary figure-8 Effect of phosphate buffer concentration on kinetic degradation of ATL in UV/EO



Supplementary figure-9 Effect of ATL concentrations on kinetic degradation of ATL in UV/EO



Supplementary figure-10 Effect of pH on kinetic degradation of ATL in UV/EO